Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

MD simulation of PE-CNT nanocomposite

Kim, Yae Ji, kim758@purdue.edu; Strachan, Alejandro, Purdue University, United States

ABSTRACT

Polymer matrix composite reinforced with carbon nanotubes (CNTs) have been received significant attention due to their potential for exceptional mechanical, electrical, thermal, and optical properties. The enhancement of ultimate mechanical properties of CNT reinforced polymer composites is governed not just by the properties of the two phases but by spatial arrangement of the CNTs, their interfaces with the matrix, and the local changes in the polymer structure and properties in the vicinity of the CNTs. We use molecular dynamics simulations to characterize the effective interaction between CNTs via the polymer matrix that govern their aggregation. We find that the short-range interaction is governed by the interactions between the perturbations the CNTs cause on the polymer density. We also quantify how these short range perturbations of the polymer structure affects their local mechanical response and that of the composite as a whole.